

## ON THE STABILIZATION SIZE OF SEMI-IMPLICIT FOURIER-SPECTRAL METHODS FOR 3D CAHN–HILLIARD EQUATIONS\*

DONG LI<sup>†</sup> AND ZHONGHUA QIAO<sup>‡</sup>

**Abstract.** The stabilized semi-implicit time-stepping method is an efficient algorithm to simulate phase field problems with fourth order dissipation. We consider the 3D Cahn–Hilliard equation and prove unconditional energy stability of the corresponding stabilized semi-implicit Fourier spectral scheme independent of the time step. We do not impose any Lipschitz-type assumption on the non-linearity. It is shown that the size of the stabilization term depends only on the initial data and the diffusion coefficient. Unconditional Sobolev bounds of the numerical solution are obtained and the corresponding error analysis under nearly optimal regularity assumptions is established.

**Keywords.** Cahn–Hilliard, energy stable, large time stepping, semi-implicit.

**AMS subject classifications.** 35Q35, 65M15, 65M70.

### 1. Introduction

The Cahn–Hilliard (CH) equation was introduced in [4] to describe the complicated phase separation and coarsening phenomena in non-uniform systems of binary composition such as alloys, glasses, and polymer mixtures. After non-dimensionalization of units, the equation takes the form

$$\begin{cases} \partial_t u = \Delta(-\nu \Delta u + f(u)), & (x, t) \in \Omega \times (0, \infty), \\ u|_{t=0} = u_0, \end{cases} \quad (1.1)$$

where  $u = u(x, t)$  is a real-valued function and represents the perturbation of the concentration of one of the phases. The function  $f(u)$  is given by

$$f(u) = u^3 - u = F'(u), \quad F(u) = \frac{1}{4}(u^2 - 1)^2.$$

Typically  $u = \pm 1$  corresponds to the formation of domains. The parameter  $\nu > 0$  is the diffusion coefficient and  $\sqrt{\nu}$  is the typical length scale of the transition regions between domains. When  $0 < \nu \ll 1$ , the dynamics of equation (1.1) is close to a limiting Hele–Shaw (Mullins–Sekerka) problem after some transient time. In this note we fix the spatial domain to be the usual  $2\pi$ -periodic torus  $\mathbb{T}^3 = \mathbb{S}^1 \times \mathbb{S}^1 \times \mathbb{S}^1$ ,  $\mathbb{S}^1 = \mathbb{R}/2\pi\mathbb{Z}$ . However our analysis is not limited to the periodic case and can be generalized to other boundary conditions such as bounded domain with Neumann boundary conditions.

For smooth solutions to equation (1.1), the mass conservation law takes the form

$$\frac{d}{dt} \int_{\Omega} u(x, t) dx \equiv 0. \quad (1.2)$$

---

\*Received: April 13, 2016; accepted; September 8, 2016. Communicated by Jie Shen.

D. Li was supported by an Nserc discovery grant. The research of Z. Qiao is partially supported by the Hong Kong Research Grant Council GRF grants 202112, 15302214 and NSFC/RGC Joint Research Scheme N\_HKBU204/12.

<sup>†</sup>Department of Mathematics, University of British Columbia, 1984 Mathematics Road, Vancouver, BC, Canada V6T 1Z2, (dli@math.ubc.ca) and Department of Mathematics, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, (madli@ust.hk).

<sup>‡</sup>Department of Applied Mathematics, The Hong Kong Polytechnic University, Hung Hom, Hong Kong (zhonghua.qiao@polyu.edu.hk).

Clearly, if  $\int_{\Omega} u_0(x) dx = 0$  then the same holds for  $u(x, t)$ . In this note we shall only consider initial data  $u_0$  with mean zero. Since the Fourier coefficient  $\hat{u}(0, t) \equiv 0$ , it is then possible to define the fractional Laplacian operators  $|\nabla|^s = (-\Delta)^{s/2}$  for  $s < 0$ . The Ginzburg–Landau type energy functional  $E(u)$  associated with equation (1.1) is

$$\begin{aligned} E(u) &= \int_{\Omega} \left( \frac{1}{2} \nu |\nabla u|^2 + F(u) \right) dx \\ &= \int_{\Omega} \left( \frac{1}{2} \nu |\nabla u|^2 + \frac{1}{4} (u^2 - 1)^2 \right) dx. \end{aligned} \quad (1.3)$$

Equation (1.1) is a natural gradient flow of  $E(u)$  in  $\dot{H}^{-1}$  (see equation (1.9)), i.e.

$$\partial_t u = - \left. \frac{\delta E}{\delta u} \right|_{\dot{H}^{-1}} = \Delta \left( \frac{\delta E}{\delta u} \right),$$

where  $\left. \frac{\delta E}{\delta u} \right|_{\dot{H}^{-1}}$ ,  $\frac{\delta E}{\delta u}$  denote the usual variational derivatives in  $\dot{H}^{-1}$  and  $L^2$  respectively. From this (and noting that  $\partial_t u$  has mean zero), one can derive the basic energy identities

$$\begin{aligned} \frac{d}{dt} E(u(t)) + \| |\nabla|^{-1} \partial_t u \|_2^2 &= 0, \\ \frac{d}{dt} E(u(t)) + \int_{\Omega} |\nabla(-\nu \Delta u + f(u))|^2 dx &= 0. \end{aligned}$$

It follows easily that  $E(u(t_2)) \leq E(u(t_1))$  for any  $0 \leq t_1 \leq t_2 < \infty$ . This then gives an a priori  $H^1$ -bound on the solution. By a scaling analysis the critical space (in 3D) for equation (1.1) is  $H^{\frac{1}{2}}$ . Global wellposedness of equation (1.1) in  $H^1$  then follows easily from these considerations and standard arguments.

The numerical simulation and analysis of the CH equation and related phase field models have been intensively investigated in the past several decades, see, e.g., [3, 5, 7, 8, 13, 15, 24, 31, 32, 6, 12, 16, 19, 20, 22, 23, 29, 14] and the references therein. Feng and Prohl [9] established error analysis of a semi-discrete (in time) and fully discrete finite element method for CH. In [28], by using the method of reduction of order, Sun derived a second order accurate linearized finite difference scheme and proved the error bound (in discrete  $L^2$  norm)  $O(\Delta x^2 + \Delta y^2 + \Delta t^2)$ . Chen and Shen [5] considered a semi-implicit Fourier-spectral scheme for equation (1.1)

$$\frac{\widehat{u^{n+1}}(k) - \widehat{u^n}(k)}{\Delta t} = -\nu |k|^4 \widehat{u^{n+1}}(k) - |k|^2 \widehat{f(u^n)}(k). \quad (1.4)$$

Note that the linear part is treated implicitly and the nonlinear part is evaluated explicitly which is a typical feature of semi-implicit methods. It is known that the semi-implicit schemes can generate large truncation errors and lose energy stability for large time steps. As a result smaller time steps are usually enforced for schemes such as equation (1.4). To resolve this issue, a class of stabilized semi-implicit methods were proposed in [11, 15, 24, 30, 32]. A notable feature of these methods is that larger time steps can be taken without losing energy stability. The basic idea is to add an additional  $O(\Delta t)$  stabilizing term to the numerical scheme to alleviate the time step constraint. In [32] the authors considered the Fourier spectral approximation of the modified Cahn–Hilliard–Cook equation

$$\partial_t C = \nabla \cdot \left( (1 - aC^2) \nabla (C^3 - C - \kappa \nabla^2 C) \right), \quad (1.5)$$

and used a stabilization term of the form

$$-A\Delta^2(C^{n+1} - C^n),$$

where  $C^n$  is the numerical solution. Note that such a term formally scales as  $O(\Delta t)$ . In [15], He, Liu and Tang considered a stabilized semi-implicit Fourier spectral scheme for the CH model, with an  $O(\Delta t)$  stabilization term

$$A\Delta(u^{n+1} - u^n).$$

The energy stability  $E(u^{n+1}) \leq E(u^n)$  is proved under a condition on  $A$  of the form

$$A \geq \max_{x \in \Omega} \left\{ \frac{1}{2}|u^n(x)|^2 + \frac{1}{4}|u^{n+1}(x) + u^n(x)|^2 \right\} - \frac{1}{2}, \quad \text{for all } n \geq 0. \quad (1.6)$$

Note that the bound of  $A$  is conditional. In particular it depends on the numerical solution itself, which implicitly has a dependence on  $A$  as well.

To obtain energy stability without any a priori assumption on the numerical solution, a different idea was pursued in [24], where Shen and Yang considered the Allen–Cahn and CH equations with truncated nonlinearity. This idea came from the remarkable observation that in practical numerical simulations the numerical solutions always stay well bounded and the nonlinear term coincides with a truncated nonlinearity effectively. By assuming

$$\max_{u \in \mathbb{R}} |\tilde{f}'(u)| \leq L,$$

where  $\tilde{f}(u)$  is a suitable truncation of the original function  $f(u)$ , Shen and Yang proved unconditional energy stability for both Allen–Cahn and CH equations. Similar assumption was used recently in [11] for the analysis of stabilized Crank–Nicolson or Adams–Bashforth scheme for Allen–Cahn and CH equations.

From the analysis point of view, the prior analytical developments are conditional and somewhat unsatisfactory in the sense that either one makes a Lipschitz assumption on the nonlinear term, or one assumes certain a priori  $L^\infty$  bounds on the numerical solution. It is thus very desirable to remove these technical restrictions and prove unconditional energy stability of stabilized large time stepping semi-implicit numerical schemes for general phase field models. In our recent work [18], we first considered the stabilized semi-implicit Fourier spectral methods for 2D phase field models including the CH and thin film equations. By using harmonic analysis in borderline spaces ([1, 2, 17]) and developing a new bootstrap scheme, we proved unconditional energy stability and characterized the size of the stability parameter as a function of the diffusion coefficient and the initial data. In the second order (in time) case [20], we further developed several new stabilization techniques to prove unconditional and conditional stability, and in the latter case we identified (almost sharp) stability region for the corresponding stabilization parameters. Note that with respect to  $L^\infty$  bound, 2D is critical thanks to the energy conservation which yields an a priori  $H^1$  bound. In fact it is well known that  $H^1$  fails to embed into  $L^\infty$  in 2D by a logarithm factor. On the other hand for 3D CH the  $H^1$  bound is clearly insufficient to yield  $L^\infty$  control and more work is needed to achieve energy stability. The purpose of this note is to settle the 3D case.

We now state the main results. Consider the stabilized semi-implicit scheme introduced in [15, 30]:

$$\begin{cases} \frac{u^{n+1} - u^n}{\tau} = -\nu\Delta^2 u^{n+1} + A\Delta(u^{n+1} - u^n) + \Delta\Pi_N(f(u^n)), & n \geq 0, \\ u^0 = \Pi_N u_0. \end{cases} \quad (1.7)$$

where  $\tau > 0$  denotes the time step, and  $A > 0$  controls the “strength” of the  $O(\tau)$  stabilization term. For any  $k = (k_1, k_2, k_3) \in \mathbb{Z}^3$ , define

$$|k|_\infty = \max\{|k_1|, |k_2|, |k_3|\}.$$

For each integer  $N \geq 2$ , introduce the space  $X_N$  as

$$X_N = \text{span}\left\{\cos(k \cdot x), \sin(k \cdot x) : |k|_\infty \leq N, k \in \mathbb{Z}^3\right\}.$$

In practical numerical simulations,  $(N + 1)$  is usually taken to be a dyadic number so that the Fast Fourier Transform method can be implemented. The  $L^2$  projection operator  $\Pi_N : L^2(\Omega) \rightarrow X_N$  is defined via the relation

$$(\Pi_N u - u, \phi) = 0, \quad \forall \phi \in X_N, \tag{1.8}$$

where  $(\cdot, \cdot)$  denotes the usual  $L^2$  inner product on  $\Omega$ . Alternatively, if  $u$  has the Fourier expansion

$$u(x) = \frac{1}{(2\pi)^3} \sum_{k \in \mathbb{Z}^3} \hat{u}(k) e^{ik \cdot x},$$

then

$$(\Pi_N u)(x) = \frac{1}{(2\pi)^3} \sum_{\substack{|k|_\infty \leq N \\ k \in \mathbb{Z}^3}} \hat{u}(k) e^{ik \cdot x}.$$

Since  $u^0 \in X_N$ , by an easy induction argument, we have  $u^n \in X_N$  for all  $n \geq 0$ . Also since the initial data  $u_0$  has mean zero,  $u^n$  has mean zero for all  $n \geq 0$ .

**THEOREM 1.1** (Unconditional energy stability for 3D CH). *Consider scheme (1.7) with  $\nu > 0$ . Assume  $u_0 \in H^2(\Omega)$  with mean zero. Denote  $E_0 = E(u_0)$  the initial energy. There exists a constant  $\beta_c > 0$  depending only on  $E_0$  such that if*

$$A \geq \beta \cdot (\|u_0\|_{H^2}^2 + \nu^{-3} + 1), \quad \beta \geq \beta_c,$$

then

$$E(u^{n+1}) \leq E(u^n), \quad \forall n \geq 0,$$

where

$$E(u) = \int_\Omega \left( \frac{1}{2} \nu |\nabla u|^2 + \frac{1}{4} (u^2 - 1)^2 \right) dx.$$

**REMARK 1.1.** It is worth emphasizing that the above stability result is unconditional in the sense that it does not depend on the time step  $\tau$ . In particular the stabilization size  $A$  is independent of  $\tau$ . In the 2D case, the condition on  $A$  (see Theorem 1.1 in [18]) takes the form

$$A \geq \beta \cdot (\|u_0\|_{H^2}^2 + \nu^{-1} |\log \nu|^2 + 1),$$

which is weaker in terms of the dependence on  $\nu$ . In the present 3D case, the condition on  $A$  is stronger due to the lack of  $L^\infty$ -control already alluded to earlier. Note that

the lower bound on  $A$  deteriorates as  $\nu \rightarrow 0$ . A more satisfactory result would involve a bound weakly dependent on  $\nu$ . Nevertheless Theorem 1.1 is a first result in this direction for the 3D case.

For the error estimate we have the following theorem.

**THEOREM 1.2** ( $L^2$  error estimate for CH). *Let  $\nu > 0$ . Let  $u_0 \in H^s$ ,  $s \geq 4$  with mean zero. Let  $u(t)$  be the solution to the 3D CH equation (1.1) with initial data  $u_0$ . Let  $u^n$  be defined according to equation (1.7) with initial data  $u^0 = \Pi_N u_0$ . Assume  $A$  satisfies the same condition in Theorem 1.1. Define  $t_m = m\tau$ ,  $m \geq 1$ . Then*

$$\|u(t_m) - u^m\|_2 \leq C_1 e^{C_2 t_m} \cdot (N^{-s} + \tau),$$

where  $C_1 > 0$ ,  $C_2 > 0$  are constants depending on  $(u_0, \nu, s, A)$ .

**REMARK 1.2.** By interpolating with the  $H^s$  Sobolev estimates on  $u^n$  (see Section 3) and the PDE solution  $u$ , we can also obtain error estimates for  $\|u(t_m) - u^m\|_{H^{s'}}$  for  $0 < s' < s$ . Alternatively one can work directly with  $H^{s'}$  error estimates and get better results in terms of dependence on the time step  $\tau$ . However we shall not pursue such results here since these higher order spaces are not physically relevant from the point of view of studying pattern formation and coarsening phenomena.

**REMARK 1.3.** To keep the argument simple, we did not make it explicit the dependence of the constants  $C_1, C_2$  on the parameter  $A$ . A close inspection of our proof reveals that  $C_1, C_2$  are monotonically increasing function of  $A$ . This is somewhat expected since the stabilization term contributes to truncation errors. In the 2D case, we showed that (see Theorem 1.3 in [18])

$$\|u(t_m) - u^m\|_2 \leq A \cdot e^{C_1 t_m} \cdot C_2 \cdot (N^{-s} + \tau),$$

where  $C_1 > 0$  depends only on  $(u_0, \nu)$ , and  $C_2 > 0$  depends on  $(u_0, \nu, s)$ . Such a result is possible thanks to the fact that in 2D  $H^1$  shares the same scaling as  $L^\infty$ , and only  $L^\infty$  bounds of the PDE solution, and  $H^1$  bounds on the numerical solution enter the error analysis. In the present 3D scenario,  $H^1$  is no longer sufficient to give  $L^\infty$  control, and we have to prove unconditional uniform higher Sobolev bounds on the numerical solution. See Section 3 for more details.

We end this introduction by collecting some notation and preliminaries used in this note.

We denote by  $\mathbb{T}^d = \mathbb{R}^d / 2\pi\mathbb{Z}^d$  the  $2\pi$ -periodic torus.

Let  $\Omega = \mathbb{T}^d$ . For any function  $f : \Omega \rightarrow \mathbb{R}$ , we use  $\|f\|_{L^p} = \|f\|_{L^p(\Omega)}$  or sometimes  $\|f\|_p$  to denote the usual Lebesgue  $L^p$  norm for  $1 \leq p \leq \infty$ .

For any two quantities  $X$  and  $Y$ , we denote  $X \lesssim Y$  if  $X \leq CY$  for some constant  $C > 0$ . Similarly  $X \gtrsim Y$  if  $X \geq CY$  for some  $C > 0$ . We denote  $X \sim Y$  if  $X \lesssim Y$  and  $Y \lesssim X$ . The dependence of the constant  $C$  on other parameters or constants are usually clear from the context and we will often suppress this dependence. We denote  $X \lesssim_{Z_1, \dots, Z_m} Y$  if  $X \leq CY$  where the constant  $C$  depends on the parameters  $Z_1, \dots, Z_m$ .

We use the following convention for Fourier expansion on  $\Omega = \mathbb{T}^d$ :

$$(\mathcal{F}f)(k) = \hat{f}(k) = \int_{\Omega} f(x) e^{-ix \cdot k} dx, \quad f(x) = \frac{1}{(2\pi)^d} \sum_{k \in \mathbb{Z}^d} \hat{f}(k) e^{ik \cdot x}.$$

The usual Parseval then reads

$$\int_{\Omega} |f(x)|^2 dx = \frac{1}{(2\pi)^d} \sum_{k \in \mathbb{Z}^d} |\hat{f}(k)|^2.$$

For  $f : \mathbb{T}^d \rightarrow \mathbb{R}$  and  $s \geq 0$ , we define the  $H^s$ -norm and  $\dot{H}^s$ -norm of  $f$  as

$$\begin{aligned} \|f\|_{H^s}^2 &= \frac{1}{(2\pi)^d} \sum_{k \in \mathbb{Z}^d} (1 + |k|^{2s}) |\hat{f}(k)|^2, \\ \|f\|_{\dot{H}^s}^2 &= \frac{1}{(2\pi)^d} \sum_{k \in \mathbb{Z}^d} |k|^{2s} |\hat{f}(k)|^2. \end{aligned} \tag{1.9}$$

provided the above series converge. In particular for  $s = 1$

$$\|f\|_{\dot{H}^1} = \|\nabla f\|_2.$$

If  $f$  has mean zero, then  $\hat{f}(0) = 0$  and clearly

$$\|f\|_{H^s} \sim \left( \sum_{k \in \mathbb{Z}^d} |k|^{2s} |\hat{f}(k)|^2 \right)^{\frac{1}{2}}.$$

For  $f$  with mean zero, one can define the  $\dot{H}^s$ -norm for  $s < 0$  by

$$\|f\|_{\dot{H}^s} = \left( \frac{1}{(2\pi)^d} \sum_{0 \neq k \in \mathbb{Z}^d} |k|^{2s} |\hat{f}(k)|^2 \right)^{\frac{1}{2}}$$

provided the series converges.

For mean zero functions, we can define the fractional Laplacian  $|\nabla|^s = (-\Delta)^{s/2}$ ,  $s \in \mathbb{R}$  by the relation

$$\widehat{|\nabla|^s f}(k) = |k|^s \hat{f}(k), \quad 0 \neq k \in \mathbb{Z}^d. \tag{1.10}$$

The mean zero condition is only needed for  $s < 0$ . For any  $s \in \mathbb{R}$ , we will use the notation  $\langle \nabla \rangle^s = (1 - \Delta)^{s/2}$  which corresponds to the Fourier multiplier  $(1 + |k|^2)^{s/2}$ .

We shall use the following simple interpolation inequalities.

LEMMA 1.1. *For any  $f \in \dot{H}^{-1}(\mathbb{T}^3) \cap \dot{H}^1(\mathbb{T}^3)$ , we have*

$$\|f\|_2 \leq \| |\nabla|^{-1} f \|_2^{\frac{1}{2}} \| \nabla f \|_2^{\frac{1}{2}}.$$

*For any  $f \in H^2(\mathbb{T}^3)$  with zero mean, we have*

$$\|f\|_{\infty} \lesssim \| \nabla f \|_2^{\frac{1}{2}} \| \Delta f \|_2^{\frac{1}{2}}.$$

*Proof.* The first inequality follows easily from the identity (note that  $f$  has mean zero by assumption)

$$\int f^2 dx = \int |\nabla| f \cdot |\nabla|^{-1} f dx.$$

For the second inequality, we note

$$\begin{aligned} \|f\|_{L^\infty(\mathbb{T}^3)} &\lesssim \sum_{0 \neq k \in \mathbb{Z}^3} |\hat{f}(k)| \\ &\lesssim \sum_{0 \neq |k| \leq R} |k|^{-1} \cdot |k| \cdot |\hat{f}(k)| + \sum_{|k| > R} |\hat{f}(k)| \cdot |k|^2 \cdot |k|^{-2} \\ &\lesssim \|\nabla f\|_2 \cdot \left( \sum_{0 < |k| \leq R} |k|^{-2} \right)^{\frac{1}{2}} + \|\Delta f\|_2 \cdot \left( \sum_{|k| > R} |k|^{-4} \right)^{\frac{1}{2}} \\ &\lesssim \|\nabla f\|_2 \cdot R^{\frac{1}{2}} + R^{-\frac{1}{2}} \|\Delta f\|_2. \end{aligned}$$

Optimizing  $R$  then yields the result. □

**2. Proof of the stability result**

In this section, we will give the proof for the stability result, i.e. Theorem 1.1.

**2.1. Proof of Theorem 1.1.** We first rewrite equation (1.7) as

$$\begin{cases} u^{n+1} = \frac{1 - A\tau\Delta}{1 + \nu\tau\Delta^2 - A\tau\Delta} u^n + \frac{\tau\Delta\Pi_N}{1 + \nu\tau\Delta^2 - A\tau\Delta} f(u^n), & n \geq 0; \\ u^0 = \Pi_N u_0. \end{cases} \tag{2.1}$$

Note that by definition  $u^0$  is a Fourier truncation of  $u_0$  and in general  $E(u^0) \neq E(u_0)$ . The following proposition clarifies this point.

**PROPOSITION 2.1** (Relation between  $E(\Pi_N u_0)$  and  $E(u_0)$ ). *For any  $u_0 \in H^1(\mathbb{T}^3)$ , we have*

- 1)  $\lim_{N \rightarrow \infty} E(\Pi_N u_0) = E(u_0)$ ;
- 2)  $\sup_{N \geq 1} E(\Pi_N u_0) \lesssim 1 + E(u_0)$ .

*Proof.* Since  $\|\nabla \Pi_N u_0\|_2 \leq \|\nabla u_0\|_2$  and  $\lim_{N \rightarrow \infty} \|\nabla \Pi_N u_0\|_2 = \|\nabla u_0\|_2$ , we only need to check the potential energy (i.e.  $F(u) = (u^2 - 1)^2/4$ ) part. Now denoting  $\Pi_{>N} = \text{Id} - \Pi_N$ , we have

$$\begin{aligned} & \left| \int ((\Pi_N u_0)^2 - 1)^2 dx - \int ((u_0)^2 - 1)^2 dx \right| \\ & \lesssim \|\Pi_N u_0 - u_0\|_4 \cdot (\|\Pi_N u_0\|_4 + \|u_0\|_4) \cdot (\|\Pi_N u_0\|_4^2 + \|u_0\|_4^2 + 1) \\ & \lesssim \|\Pi_{>N} u_0\|_{H^1} \cdot (1 + \|u_0\|_{H^1}^3) \rightarrow 0, \quad \text{as } N \rightarrow \infty. \end{aligned}$$

Thus 1) holds.

For 2) we only need to check the inequality

$$\sup_{N \geq 1} \|\Pi_N u_0\|_4 \lesssim \|u_0\|_4.$$

But this follows easily from the fact that  $\Pi_N$  is the product of one-dimensional Hilbert-type transforms. (Recall that  $\widehat{\Pi_N}(k_1, k_2, k_3) = \prod_{j=1}^3 \chi_N(k_j)$ ,  $\chi_N = \chi_{(-\infty, N]} - \chi_{(-\infty, -N]}$ , and  $\chi$  is the usual characteristic function.) □

LEMMA 2.1. *Suppose  $E(u^n) \leq B$  for some  $B > 0$ , then*

$$\left\| \frac{1 - A\tau\Delta}{1 + \nu\tau\Delta^2 - A\tau\Delta} u^n \right\|_{\dot{H}^2(\mathbb{T}^3)} \lesssim_B A^{\frac{1}{2}} \nu^{-\frac{1}{2}} + (A\tau\nu)^{-\frac{1}{2}}.$$

*Proof.* To ease the notation we shall write  $\lesssim_B$  simply as  $\lesssim$ . Clearly

$$\left\| \frac{1 - A\tau\Delta}{1 + \nu\tau\Delta^2 - A\tau\Delta} u^n \right\|_{\dot{H}^2(\mathbb{T}^3)} \lesssim \left\| \frac{(1 + A\tau|k|^2)|k|^2}{1 + \nu\tau|k|^4 + A\tau|k|^2} \widehat{u}^n(k) \right\|_{l_k^2(\mathbb{Z}^3)} =: X.$$

Here for any  $h: \mathbb{Z}^3 \rightarrow \mathbb{C}$ , we denote

$$\|h\|_{l_k^2(\mathbb{Z}^3)} = \left( \sum_{k \in \mathbb{Z}^3} |h(k)|^2 \right)^{\frac{1}{2}}.$$

Now discuss several cases.

If  $A\tau|k|^2 \leq 1$ , then

$$\begin{aligned} X &\lesssim \| |k|^2 \widehat{u}^n(k) \|_{l_k^2(k \in \mathbb{Z}^3: |k| \leq \sqrt{\frac{1}{A\tau}})} \\ &\lesssim (A\tau)^{-\frac{1}{2}} \|u^n\|_{\dot{H}^1} \lesssim (A\tau\nu)^{-\frac{1}{2}}. \end{aligned}$$

If  $A\tau|k|^2 > 1$  and  $\nu\tau|k|^4 \leq A\tau|k|^2$  (i.e.  $|k|^2 \leq \frac{A}{\nu}$ ), then

$$\begin{aligned} X &\lesssim \| |k|^2 \widehat{u}^n(k) \|_{l_k^2(k \in \mathbb{Z}^3: |k| \leq \sqrt{\frac{A}{\nu}})} \\ &\lesssim \sqrt{\frac{A}{\nu}} \cdot \|u^n\|_{\dot{H}^1} \lesssim A^{\frac{1}{2}} \nu^{-1}. \end{aligned}$$

If  $A\tau|k|^2 > 1$  and  $\nu\tau|k|^4 > A\tau|k|^2$  (i.e.  $|k|^2 > \frac{A}{\nu}$ ), then

$$\begin{aligned} X &\lesssim \left\| \frac{A\tau|k|^4}{\nu\tau|k|^4} \widehat{u}^n(k) \right\|_{l_k^2(k \in \mathbb{Z}^3: |k| > \sqrt{\frac{A}{\nu}})} \\ &\lesssim \frac{A}{\nu} \cdot \| |k|^{-1} |k| \widehat{u}^n(k) \|_{l_k^2(k \in \mathbb{Z}^3: |k| > \sqrt{\frac{A}{\nu}})} \\ &\lesssim \sqrt{\frac{A}{\nu}} \cdot \|u^n\|_{\dot{H}^1} \lesssim A^{\frac{1}{2}} \nu^{-1}. \end{aligned}$$

□

LEMMA 2.2. *Suppose  $E(u^n) \leq B$ , then for  $u^{n+1}$  we have*

$$\begin{aligned} \|u^{n+1}\|_{\dot{H}^2(\mathbb{T}^3)} &\lesssim_B (A^{\frac{1}{2}} + 1)\nu^{-1} + (A\tau\nu)^{-\frac{1}{2}} + \nu^{-\frac{5}{2}}, \\ \|u^{n+1}\|_{\dot{H}^1(\mathbb{T}^3)} &\lesssim_B \nu^{-\frac{1}{2}} + A^{-\frac{1}{2}}\nu^{-2} + A^{-\frac{1}{2}}\nu^{-\frac{1}{2}}, \\ \|u^{n+1}\|_{L^\infty(\mathbb{T}^3)}^2 &\leq \alpha_B \cdot (\nu^{-\frac{1}{2}} + A^{-\frac{1}{2}}\nu^{-2} + A^{-\frac{1}{2}}\nu^{-\frac{1}{2}}) \cdot ((A^{\frac{1}{2}} + 1)\nu^{-1} + (A\tau\nu)^{-\frac{1}{2}} + \nu^{-\frac{5}{2}}), \end{aligned}$$

where  $\alpha_B > 0$  is a constant depending only on  $B$ .

*Proof.* We shall write  $\lesssim_B$  as  $\lesssim$ . By Lemma 2.1 and observing that

$$\sup_{k \in \mathbb{Z}^3} \frac{\tau|k|^4}{1 + \nu\tau|k|^4 + A\tau|k|^2} \lesssim \frac{1}{\nu},$$



we get

$$\|u^{n+1}\|_{\dot{H}^2(\mathbb{T}^3)} \lesssim A^{\frac{1}{2}}\nu^{-1} + (A\tau\nu)^{-\frac{1}{2}} + \frac{1}{\nu}\|(u^n)^3 - u^n\|_2.$$

By Sobolev embedding (and noting that  $u^n$  has mean zero), we have

$$\|(u^n)^3\|_2 \lesssim \|u^n\|_6^3 \lesssim \|\nabla u^n\|_2^3 \lesssim \nu^{-\frac{3}{2}}.$$

Therefore

$$\|u^{n+1}\|_{\dot{H}^2(\mathbb{T}^3)} \lesssim (A^{\frac{1}{2}} + 1)\nu^{-1} + (A\tau\nu)^{-\frac{1}{2}} + \nu^{-\frac{5}{2}}.$$

For the  $\dot{H}^1$  bound, note that

$$\sup_{k \in \mathbb{Z}^3} \frac{\tau|k|^3}{1 + \nu\tau|k|^4 + A\tau|k|^2} \lesssim \sup_{k \in \mathbb{Z}^3} \frac{\tau|k|^3}{1 + 2\tau\sqrt{A\nu}|k|^3} \lesssim (A\nu)^{-\frac{1}{2}}.$$

Therefore

$$\begin{aligned} \|u^{n+1}\|_{\dot{H}^1(\mathbb{T}^3)} &\lesssim \|u^n\|_{\dot{H}^1} + (A\nu)^{-\frac{1}{2}}\|(u^n)^3 - u^n\|_2 \\ &\lesssim \nu^{-\frac{1}{2}} + (A\nu)^{-\frac{1}{2}} \cdot (\nu^{-\frac{3}{2}} + 1) \\ &\lesssim \nu^{-\frac{1}{2}} + A^{-\frac{1}{2}}\nu^{-2} + A^{-\frac{1}{2}}\nu^{-\frac{1}{2}}. \end{aligned}$$

Finally to bound  $\|u^{n+1}\|_\infty$ , we just use the interpolation inequality (for  $h$  with mean zero, see Lemma 1.1)

$$\|h\|_{L^\infty(\mathbb{T}^3)} \lesssim \|h\|_{\dot{H}^1(\mathbb{T}^3)}^{\frac{1}{2}} \|h\|_{\dot{H}^2(\mathbb{T}^3)}^{\frac{1}{2}}.$$

□

LEMMA 2.3. For any  $n \geq 0$ ,

$$\begin{aligned} &E(u^{n+1}) - E(u^n) + \left( A + \frac{1}{2} + \sqrt{\frac{2\nu}{\tau}} \right) \|u^{n+1} - u^n\|_2^2 \\ &\leq \|u^{n+1} - u^n\|_2^2 \cdot \frac{3}{2} \left( \|u^n\|_\infty^2 + \|u^{n+1}\|_\infty^2 \right). \end{aligned} \tag{2.2}$$

REMARK 2.1. A better bound is  $\|u^{n+1} - u^n\|_2^2 \cdot (\|u^n\|_\infty^2 + \frac{1}{2}\|u^{n+1}\|_\infty^2)$ , but we do not need such improvement in our analysis later.

*Proof.* We shall denote by  $(\cdot, \cdot)$  the usual  $L^2$  inner product. Recall

$$\frac{u^{n+1} - u^n}{\tau} = -\nu\Delta^2 u^{n+1} + A\Delta(u^{n+1} - u^n) + \Delta\Pi_N f(u^n).$$

Taking the  $L^2$  inner product with  $(-\Delta)^{-1}(u^{n+1} - u^n)$  on both sides and using the identity

$$b \cdot (b - a) = \frac{1}{2}(|b|^2 - |a|^2 + |b - a|^2), \quad \forall a, b \in \mathbb{R}^d, \tag{2.3}$$

we get

$$\begin{aligned} \frac{1}{\tau} \|\nabla|^{-1}(u^{n+1} - u^n)\|_2^2 + \frac{\nu}{2} (\|\nabla u^{n+1}\|_2^2 - \|\nabla u^n\|_2^2 + \|\nabla(u^{n+1} - u^n)\|_2^2) \\ + A\|u^{n+1} - u^n\|_2^2 = -(f(u^n), u^{n+1} - u^n). \end{aligned} \tag{2.4}$$

Define  $g(s) = F(u^n + s(u^{n+1} - u^n))$  (recall  $F' = f$ ). By using the Taylor expansion

$$g(1) = g(0) + g'(0) + \int_0^1 g''(s)(1-s)ds,$$

we get

$$\begin{aligned} F(u^{n+1}) = F(u^n) + f(u^n)(u^{n+1} - u^n) - \frac{1}{2}(u^{n+1} - u^n)^2 \\ + (u^{n+1} - u^n)^2 \cdot \int_0^1 \tilde{f}(u^n + s(u^{n+1} - u^n))(1-s)ds, \end{aligned}$$

where  $\tilde{f}(z) = 3z^2$ .

We then obtain

$$\begin{aligned} E(u^{n+1}) - E(u^n) + \frac{1}{\tau} \|\nabla|^{-1}(u^{n+1} - u^n)\|_2^2 + (A + \frac{1}{2})\|u^{n+1} - u^n\|_2^2 \\ \leq \|u^{n+1} - u^n\|_2 \cdot \frac{3}{2} (\|u^n\|_\infty^2 + \|u^{n+1}\|_\infty^2). \end{aligned}$$

The result then follows from the inequalities (see Lemma 1.1)

$$\begin{aligned} \frac{1}{\tau} \|\nabla|^{-1}(u^{n+1} - u^n)\|_2^2 + \frac{\nu}{2} \|\nabla(u^{n+1} - u^n)\|_2^2 \\ \geq \sqrt{\frac{2\nu}{\tau}} \|\nabla|^{-1}(u^{n+1} - u^n)\|_2 \|\nabla(u^{n+1} - u^n)\|_2 \geq \sqrt{\frac{2\nu}{\tau}} \|u^{n+1} - u^n\|_2^2. \end{aligned}$$

*Proof. (Proof of Theorem 1.1.)* Set □

$$B = \sup_{N \geq 1} E(\Pi_N u_0).$$

By Proposition 2.1, we have

$$B \lesssim 1 + E(u_0) < \infty.$$

We shall inductively prove for each  $m \geq 1$ :

$$\begin{aligned} E(u^m) \leq B, \quad E(u^m) \leq E(u^{m-1}), \\ \|u^m\|_\infty^2 \leq \alpha_B \cdot (\nu^{-\frac{1}{2}} + A^{-\frac{1}{2}}\nu^{-2} + A^{-\frac{1}{2}}\nu^{-\frac{1}{2}}) \cdot ((A^{\frac{1}{2}} + 1)\nu^{-1} + (A\tau\nu)^{-\frac{1}{2}} + \nu^{-\frac{5}{2}}), \end{aligned}$$

where  $\alpha_B > 0$  is the same constant in Lemma 2.2. The value of the parameter  $A$  will be specified in the course of the proof.

We first check the “base” case  $m = 1$ . Since  $E(u^0) \leq B$ , we can use Lemma 2.2 to get

$$\|u^1\|_\infty^2 \leq \alpha_B \cdot (\nu^{-\frac{1}{2}} + A^{-\frac{1}{2}}\nu^{-2} + A^{-\frac{1}{2}}\nu^{-\frac{1}{2}}) \cdot ((A^{\frac{1}{2}} + 1)\nu^{-1} + (A\tau\nu)^{-\frac{1}{2}} + \nu^{-\frac{5}{2}}).$$

We then only need to check  $E(u^1) \leq E(u^0)$ . By Lemma 2.3, this amounts to checking

$$A + \frac{1}{2} + \sqrt{\frac{2\nu}{\tau}} \geq \frac{3}{2} \|u^0\|_\infty^2 + \frac{3}{2} \|u^1\|_\infty^2.$$

By Sobolev embedding, we have

$$\|u^0\|_{L^\infty(\mathbb{T}^3)}^2 \leq c_1 \|u^0\|_{H^2(\mathbb{T}^3)}^2 = c_1 \|\Pi_N u_0\|_{H^2(\mathbb{T}^3)}^2 \leq c_1 \|u_0\|_{H^2(\mathbb{T}^3)}^2,$$

where  $c_1 > 0$  is an absolute constant. Thus we need to choose  $A$  such that

$$A + \frac{1}{2} + \sqrt{\frac{2\nu}{\tau}} \geq c_1 \frac{3}{2} \|u_0\|_{H^2}^2 + \frac{3}{2} \alpha_B \cdot (\nu^{-\frac{1}{2}} + A^{-\frac{1}{2}} \nu^{-2} + A^{-\frac{1}{2}} \nu^{-\frac{1}{2}}) \cdot ((A^{\frac{1}{2}} + 1)\nu^{-1} + (A\tau\nu)^{-\frac{1}{2}} + \nu^{-\frac{5}{2}}).$$

It suffices to take

$$A \geq k_B (\|u_0\|_{H^2}^2 + \nu^{-3} + 1),$$

where  $k_B > 0$  is a sufficiently large constant depending only on  $B$ .

Next we check the induction step. Assume the induction hypothesis holds for  $m = n$ . Then for  $u^{n+1}$ , by Lemma 2.2, we get

$$\|u^{n+1}\|_\infty^2 \leq \alpha_B \cdot (\nu^{-\frac{1}{2}} + A^{-\frac{1}{2}} \nu^{-2} + A^{-\frac{1}{2}} \nu^{-\frac{1}{2}}) \cdot ((A^{\frac{1}{2}} + 1)\nu^{-1} + (A\tau\nu)^{-\frac{1}{2}} + \nu^{-\frac{5}{2}}).$$

Thus we only need to show  $E(u^{n+1}) \leq E(u^n)$ . By Lemma 2.3, this in turn follows from the inequality

$$A + \frac{1}{2} + \sqrt{\frac{2\nu}{\tau}} \geq \frac{3}{2} \|u^n\|_\infty^2 + \frac{3}{2} \|u^{n+1}\|_\infty^2.$$

Therefore it suffices to take  $A$  such that

$$A + \frac{1}{2} + \sqrt{\frac{2\nu}{\tau}} \geq 3\alpha_B \cdot (\nu^{-\frac{1}{2}} + A^{-\frac{1}{2}} \nu^{-2} + A^{-\frac{1}{2}} \nu^{-\frac{1}{2}}) \cdot ((A^{\frac{1}{2}} + 1)\nu^{-1} + (A\tau\nu)^{-\frac{1}{2}} + \nu^{-\frac{5}{2}}).$$

Clearly it is enough to take

$$A \geq k_B \cdot (\|u_0\|_{H^2}^2 + \nu^{-3} + 1),$$

where  $k_B > 0$  is sufficiently large. □

### 3. Higher Sobolev bounds on the numerical solution

In this section we establish unconditional Sobolev bounds on the numerical solutions. This is given by the following proposition.

**PROPOSITION 3.1 (Unconditional Sobolev bounds).** *Suppose  $u_0 \in H^s(\mathbb{T}^3)$ ,  $s \geq 2$  with mean zero. Then*

$$\sup_{n \geq 0} \|u^n\|_{H^s} \lesssim_{\nu, A, u_0, s} 1. \tag{3.1}$$

**REMARK 3.1.** Note that the bound on  $u^n$  is independent of the time step  $\tau$  (thus the name “unconditional”) and the Galerkin truncation number  $N$ .

*Proof. (Proof of Proposition 3.1.)* Write

$$\begin{aligned}
 u^{n+1} &= \underbrace{\frac{1 - A\tau\Delta}{1 + \nu\Delta^2 - A\tau\Delta}}_{L_1} u^n + \underbrace{\frac{\tau\Delta\Pi_N}{1 + \nu\tau\Delta^2 - A\tau\Delta}}_{L_2} f(u^n) \\
 &= L_1(L_1 u^{n-1} + L_2 f(u^{n-1})) + L_2 f(u^n) \\
 &= L_1^{m_0+1} u^{n-m_0} + \sum_{l=0}^{m_0} L_1^l L_2 f(u^{n-l}),
 \end{aligned} \tag{3.2}$$

where  $m_0$  is to be chosen later.

We discuss a few cases.

Case 1:  $\tau \geq 1/10$ . Clearly for each  $0 \neq k \in \mathbb{Z}^3$ ,

$$\begin{aligned}
 |\widehat{L_1}(k)| &= \frac{1 + A\tau|k|^2}{1 + \nu\tau|k|^4 + A\tau|k|^2} \\
 &\leq \frac{1}{1 + \nu\tau|k|^4 + A\tau|k|^2} + \frac{A}{\nu|k|^2 + A} \\
 &\lesssim_{\nu,A} \frac{1}{1 + |k|^2};
 \end{aligned}$$

$$|\widehat{L_2}(k)| \leq \frac{|k|^2}{\nu|k|^4 + A|k|^2} \lesssim_{\nu,A} \frac{1}{1 + |k|^2}.$$

Therefore for any  $n \geq 0$ ,

$$\|u^{n+1}\|_{H^2} \lesssim_{\nu,A} \|u^n\|_2 + \|(u^n)^3 - u^n\|_2 \lesssim_{\nu,A,u_0} 1.$$

An iteration of this argument then easily yields bound (3.1).

Case 2:  $0 < \tau < 1/10$  and  $A\tau|k|^2 \geq 1/10$ . Then

$$\begin{aligned}
 |\widehat{L_1}(k)| &\lesssim \frac{A\tau|k|^2}{\nu\tau|k|^4 + A\tau|k|^2} \lesssim_{\nu,A} \frac{1}{1 + |k|^2}, \\
 |\widehat{L_2}(k)| &\lesssim_{\nu,A} \frac{1}{1 + |k|^2}.
 \end{aligned}$$

The bound (3.1) easily follows in this case.

Case 3:  $0 < \tau < 1/10$  and  $A\tau|k|^2 < 1/10$ . Take  $m_0$  to be the unique integer such that  $\frac{1}{2} \leq m_0\tau < 1$ . Note that  $m_0 \geq 5$ . We shall use equation (3.2). For this first observe that

$$\begin{aligned}
 |\widehat{L_1^{m_0+1}}(k)| &\leq \left( \frac{1 + A\tau|k|^2}{1 + A\tau|k|^2 + \nu\tau|k|^4} \right)^{m_0+1} \\
 &\leq \left( 1 + \frac{1}{1 + A\tau|k|^2} \nu\tau|k|^4 \right)^{-m_0} \\
 &\leq \left( 1 + \frac{1}{2} \nu|k|^4 \frac{t_0}{m_0} \right)^{-m_0},
 \end{aligned}$$

where  $t_0 = m_0\tau \in [\frac{1}{2}, 1)$ .

Now for any  $a > 0$  consider the function

$$g(x) = -x \log(1 + a/x), \quad x > 0.$$

Easy to check that

$$\begin{aligned} g'(x) &= -\log\left(1 + \frac{a}{x}\right) + \frac{a}{x+a}, \\ g''(x) &= \frac{a}{x+a} \left(\frac{1}{x} - \frac{1}{x+a}\right). \end{aligned}$$

Thus  $g(x)$  is decreasing on  $(0, \infty)$ .

Therefore it follows that

$$|\widehat{L_1^{m_0+1}}(k)| \leq \left(1 + \frac{1}{2} \nu |k|^4 \frac{t_0}{m_0}\right)^{-m_0} \leq \left(1 + \frac{1}{2} \nu |k|^4 \cdot \frac{t_0}{5}\right)^{-5}.$$

On the other hand, observe

$$\begin{aligned} |\widehat{L_2}(k)| \cdot \sum_{l=0}^{m_0} |\widehat{L_1}(k)|^l &= \frac{1 - |\widehat{L_1}(k)|^{m_0+1}}{1 - |\widehat{L_1}(k)|} |\widehat{L_2}(k)| \\ &\leq \frac{1}{1 - \frac{1+A\tau|k|^2}{1+\nu\tau|k|^4+A\tau|k|^2}} \cdot \frac{\tau|k|^2}{1 + \nu\tau|k|^4 + A\nu|k|^2} \\ &= \frac{1}{\nu\tau|k|^4} \cdot \tau|k|^2 \lesssim_\nu \frac{1}{|k|^2}. \end{aligned}$$

Therefore for  $n \geq m_0$ , by using equation (3.2), we get

$$\|u^{n+1}\|_{H^2} \lesssim_{\nu,A} \|u^{n-m_0}\|_2 + \sup_{0 \leq l \leq m_0} \|f(u^{n-l})\|_2 \lesssim_{\nu,A,u_0} 1.$$

Similarly if  $1 \leq n \leq m_0 + 1$ , then we shall use the formula

$$u^n = L_1^n u^0 + \sum_{l=0}^{n-1} L_1^l L_2 f(u^{n-1-l}).$$

Then

$$\|u^n\|_{H^2} \lesssim_\nu \|u^0\|_{H^2} + \sup_{0 \leq l \leq n-1} \|f(u^{n-1-l})\|_2 \lesssim_{\nu,A,u_0} 1.$$

An iteration of the above argument then easily yields the bound (3.1). □

#### 4. Error estimate for CH

In this section we carry out the error estimate for  $CH$  in  $L^2$ .

##### 4.1. Auxiliary $L^2$ error estimate for near solutions. Consider

$$\begin{cases} \frac{v^{n+1} - v^n}{\tau} = -\nu \Delta^2 v^{n+1} + A \Delta (v^{n+1} - v^n) + \Delta \Pi_N f(v^n), & n \geq 0, \\ \frac{\tilde{v}^{n+1} - \tilde{v}^n}{\tau} = -\nu \Delta^2 \tilde{v}^{n+1} + A \Delta (\tilde{v}^{n+1} - \tilde{v}^n) + \Delta \Pi_N f(\tilde{v}^n) - \Delta \tilde{G}^n, & n \geq 0, \\ v^0 = v_0, \quad \tilde{v}^0 = \tilde{v}_0, \end{cases} \tag{4.1}$$

where  $v_0$  and  $\tilde{v}_0$  have mean zero.

We first recall a simple lemma.

LEMMA 4.1 (Discrete Gronwall inequality). *Let  $\tau > 0$  and  $y_n \geq 0, \alpha_n \geq 0, \beta_n \geq 0$  for  $n = 0, 1, 2, \dots$ . Suppose*

$$\frac{y_{n+1} - y_n}{\tau} \leq \alpha_n y_n + \beta_n, \quad \forall n \geq 0.$$

Then for any  $m \geq 1$ , we have

$$y_m \leq \exp\left(\tau \sum_{n=0}^{m-1} \alpha_n\right) \left(y_0 + \tau \sum_{n=0}^{m-1} \beta_n\right).$$

*Proof.* See Lemma 4.1 in [18]. □

PROPOSITION 4.1. *For solutions of system (4.1), assume for some  $N_1 > 0$ ,*

$$\sup_{n \geq 0} \|v^n\|_\infty + \sup_{n \geq 0} \|\tilde{v}^n\|_\infty \leq N_1. \tag{4.2}$$

Then for any  $m \geq 1$ ,

$$\begin{aligned} & \|v^m - \tilde{v}^m\|_2^2 \\ & \leq \exp\left(m\tau \cdot \frac{(1 + 3N_1^2)^2}{\nu}\right) \cdot \left(\|v_0 - \tilde{v}_0\|_2^2 + A\tau \|\nabla(v_0 - \tilde{v}_0)\|_2^2 + \frac{\tau}{\nu} \sum_{n=0}^{m-1} \|\tilde{G}^n\|_2^2\right). \end{aligned} \tag{4.3}$$

*Proof.* Denote  $e^n = v^n - \tilde{v}^n$ . Then

$$\frac{e^{n+1} - e^n}{\tau} = -\nu \Delta^2 e^{n+1} + A \Delta(e^{n+1} - e^n) + \Delta \Pi_N(f(v^n) - f(\tilde{v}^n)) + \Delta \tilde{G}^n. \tag{4.4}$$

Taking  $L^2$ -inner product with  $e^{n+1}$  on both sides, we get

$$\begin{aligned} & \frac{1}{2\tau} (\|e^{n+1}\|_2^2 - \|e^n\|_2^2 + \|e^{n+1} - e^n\|_2^2) \\ & \quad + \nu \|\Delta e^{n+1}\|_2^2 + \frac{A}{2} (\|\nabla e^{n+1}\|_2^2 - \|\nabla e^n\|_2^2 + \|\nabla(e^{n+1} - e^n)\|_2^2) \\ & = (\tilde{G}^n, \Delta e^{n+1}) + (f(v^n) - f(\tilde{v}^n), \Delta \Pi_N e^{n+1}). \end{aligned} \tag{4.5}$$

Clearly

$$|(\tilde{G}^n, \Delta e^{n+1})| \leq \frac{\|\tilde{G}^n\|_2^2}{2\nu} + \frac{\nu}{2} \|\Delta e^{n+1}\|_2^2.$$

On the other hand, recalling  $f'(z) = 3z^2 - 1$ , we get

$$|f(v^n) - f(\tilde{v}^n)| \leq |e^n| \cdot (1 + 3N_1^2).$$

Thus

$$\begin{aligned} |(f(v^n) - f(\tilde{v}^n), \Delta \Pi_N e^{n+1})| & \leq \|e^n\|_2 \cdot \|\Delta e^{n+1}\|_2 \cdot (1 + 3N_1^2) \\ & \leq \frac{\nu}{2} \|\Delta e^{n+1}\|_2^2 + \frac{(1 + 3N_1^2)^2}{2\nu} \|e^n\|_2^2. \end{aligned}$$

Collecting the estimates, we get

$$\begin{aligned} & \frac{\|e^{n+1}\|_2^2 - \|e^n\|_2^2}{2\tau} + \frac{A}{2}(\|\nabla e^{n+1}\|_2^2 - \|\nabla e^n\|_2^2) \\ & \leq \frac{1}{2\nu}\|\tilde{G}^n\|_2^2 + \frac{(1+3N_1^2)^2}{2\nu}\|e^n\|_2^2. \end{aligned} \tag{4.6}$$

It follows that

$$\begin{aligned} & \frac{\|e^{n+1}\|_2^2 + A\tau\|\nabla e^{n+1}\|_2^2 - (\|e^n\|_2^2 + A\tau\|\nabla e^n\|_2^2)}{\tau} \\ & \leq \frac{(1+3N_1^2)^2}{\nu}\|e^n\|_2^2 + \frac{1}{\nu}\|\tilde{G}^n\|_2^2. \end{aligned}$$

The result then follows from Lemma 4.1. □

**4.2. Proof of Theorem 1.2.**

*Proof.* We shall denote by  $C$  a constant depending only on  $(\nu, u_0, s, A)$ . The value of  $C$  may vary from line to line. For simplicity we shall denote  $\lesssim_{\nu, A, u_0, s}$  as  $\lesssim$ .

We need to compare

$$\begin{cases} \frac{u^{n+1} - u^n}{\tau} = -\nu\Delta^2 u^{n+1} + A\Delta(u^{n+1} - u^n) + \Delta\Pi_N f(u^n), \\ \partial_t u = -\nu\Delta^2 u + \Delta f(u), \\ \tilde{u}^0 = \Pi_N u_0, \quad u(0) = u_0. \end{cases} \tag{4.7}$$

We first recast the PDE solution  $u$  into time-discretized form. Recall that for a one-variable function  $h = h(t)$ , we have the formulae

$$\frac{1}{\tau} \int_{t_n}^{t_{n+1}} h(t) dt = h(t_n) + \frac{1}{\tau} \int_{t_n}^{t_{n+1}} h'(t) \cdot (t_{n+1} - t) dt, \tag{4.8}$$

$$\frac{1}{\tau} \int_{t_n}^{t_{n+1}} h(t) dt = h(t_{n+1}) + \frac{1}{\tau} \int_{t_n}^{t_{n+1}} h'(t) \cdot (t_n - t) dt. \tag{4.9}$$

By using the above formulae and integrating the PDE for  $u$  on  $[t_n, t_{n+1}]$ , we get

$$\begin{aligned} & \frac{u(t_{n+1}) - u(t_n)}{\tau} \\ & = -\nu\Delta^2 u(t_{n+1}) + A\Delta(u(t_{n+1}) - u(t_n)) + \Delta\Pi_N f(u(t_n)) + \Delta\Pi_{>N} f(u(t_n)) + \Delta\tilde{G}^n, \end{aligned} \tag{4.10}$$

where  $\Pi_{>N} = \text{Id} - \Pi_N$  and

$$\tilde{G}^n = -\frac{\nu}{\tau} \int_{t_n}^{t_{n+1}} \partial_t \Delta u \cdot (t_n - t) dt + \frac{1}{\tau} \int_{t_n}^{t_{n+1}} \partial_t (f(u)) \cdot (t_{n+1} - t) dt - A \int_{t_n}^{t_{n+1}} \partial_t u dt. \tag{4.11}$$

Since  $\|\partial_t u\|_2 \lesssim \|\Delta \partial_t u\|_2$  (recall  $\partial_t u$  has mean zero), we have

$$\|\tilde{G}^n\|_2 \lesssim \int_{t_n}^{t_{n+1}} \|\partial_t \Delta u\|_2 dt + \int_{t_n}^{t_{n+1}} \|\partial_t u\|_2 dt \left( \|f'(u)\|_{L_t^\infty L_x^\infty} + A \right)$$

$$\lesssim \left( \int_{t_n}^{t_{n+1}} \|\partial_t \Delta u\|_2^2 dt \right)^{\frac{1}{2}} \cdot \sqrt{\tau}.$$

Then

$$\sum_{n=0}^{m-1} \|\tilde{G}^n\|_2^2 \lesssim \tau \int_0^{t_m} \|\partial_t \Delta u\|_2^2 dt \lesssim \tau(1+t_m).$$

Also it is easy to check that

$$\sum_{n=0}^{m-1} \|\Pi_{>N} f(u(t_n))\|_2^2 \lesssim_s N^{-2s} t_m / \tau. \tag{4.12}$$

Thus

$$\tau \sum_{n=0}^{m-1} (\|\tilde{G}^n\|_2^2 + \|\Pi_{>N} f(u(t_n))\|_2^2) \lesssim (1+t_m)(\tau^2 + N^{-2s}). \tag{4.13}$$

By Proposition 3.1, we have

$$\sup_{n \geq 0} \|u^n\|_{H^s} \lesssim 1.$$

Thus by Proposition 4.1, we get

$$\begin{aligned} \|u^m - u(t_m)\|_2^2 &\lesssim e^{Ct_m} \left( \|u_0 - \Pi_N u_0\|_2^2 + \tau \|\nabla u_0 - \nabla \Pi_N u_0\|_2^2 + (1+t_m) \cdot (N^{-2s} + \tau^2) \right) \\ &\lesssim e^{Ct_m} \left( N^{-2s} + N^{-2(s-1)} \tau + (1+t_m)(N^{-2s} + \tau^2) \right). \end{aligned}$$

Since  $s \geq 4$ , we have

$$N^{-2(s-1)} \tau \lesssim \tau^2 + N^{-4(s-1)} \lesssim \tau^2 + N^{-2s}.$$

Therefore we get

$$\|u^m - u(t_m)\|_2 \lesssim e^{Ct_m} (N^{-s} + \tau).$$

□

**5. Concluding remarks**

In this note we considered the stabilized semi-implicit Fourier spectral method for the 3D Cahn–Hilliard equation with the usual double well potential. The stabilization term is of the form  $A\Delta(u^{n+1} - u^n)$  which is formally of order  $O(\Delta t)$ . For  $A$  sufficiently large depending on the initial data and the diffusion coefficient  $\nu$ , we proved unconditional energy stability which works for any time step  $\tau > 0$ . By a bootstrap argument we obtained uniform higher Sobolev bounds on the numerical solution. These bounds are uniform and independent of the time step  $\tau$ . We establish the corresponding error estimate and quantify the error term as an explicit function of the time step  $\tau$  and the spectral Galerkin truncation number  $N$ . It is expected that our analysis can be carried over to the thin film equations, the molecular beam epitaxy (MBE) equations, the Allen–Cahn equation or other similar phase field models. For future study it is worthwhile mentioning that the analysis of general stabilization techniques such



as biharmonic stabilization  $-\Delta^2(u^{n+1} - u^n)$  or even fractional Laplacian stabilization  $-(-\Delta)^s(u^{n+1} - u^n)$  ( $s > 0$ ) is still missing at present. Also another interesting topic is to consider generalizing our analysis to other low order schemes such as spectral deferred correction methods ([10, 21]), higher order time stepping methods such as [30], phase field models with higher order dissipations ([7]), nonlinear diffusion models ([25]), and decoupled energy stable numerical schemes ([26, 27]). We plan to address these issues in the future.

## REFERENCES

- [1] J. Bourgain and D. Li, *Strong ill-posedness of the incompressible Euler equation in borderline Sobolev spaces*, *Invent. Math.*, 201(1):97–157, 2015.
- [2] J. Bourgain and D. Li, *Strong illposedness of the incompressible Euler equation in integer  $C^m$  spaces*, *Geom. Funct. Anal.*, 25(1):1–86, 2015.
- [3] A. Bertozzi, N. Ju, and H. Lu, *A biharmonic-modified forward time stepping method for fourth order nonlinear diffusion equations*, *Disc. Conti. Dyn. Sys.*, 29(4):1367–1391, 2011.
- [4] J.W. Cahn and J.E. Hilliard, *Free energy of a nonuniform system. I. Interfacial energy free energy*, *J. Chem. Phys.*, 28:258–267, 1958.
- [5] L.Q. Chen and J. Shen, *Applications of semi-implicit Fourier-spectral method to phase field equations*, *Comput. Phys. Comm.*, 108:147–158, 1998.
- [6] F. Chen and J. Shen, *Efficient energy stable schemes with spectral discretization in space for anisotropic Cahn–Hilliard systems*, *Commun. Comput. Phys.*, 13:1189–1208, 2013.
- [7] A. Christlieb, J. Jones, K. Promislow, B. Wetton, and M. Willoughby, *High accuracy solutions to energy gradient flows from material science models*, *J. Comput. Phys.*, 257:193–215, 2014.
- [8] W.M. Feng, P. Yu, S.Y. Hu, Z.K. Liu, Q. Du, and L. Q. Chen, *A Fourier spectral moving mesh method for the Cahn–Hilliard equation with elasticity*, *Commun. Comput. Phys.*, 5:582–599, 2009.
- [9] X.B. Feng and A. Prohl, *Error analysis of a mixed finite element method for the Cahn–Hilliard equation*, *Numer. Math.*, 99:47–84, 2004.
- [10] X. Feng, T. Tang, and J. Yang, *Long time numerical simulations for phase-field problems using  $p$ -adaptive spectral deferred correction methods*, *SIAM J. Sci. Comput.*, 37(1):A271–A294, 2015.
- [11] X. Feng, T. Tang, and J. Yang, *Stabilized Crank–Nicolson/Adams–Bashforth schemes for phase field models*, *East Asian J. Appl. Math.*, 3(1):59–80, 2013.
- [12] N. Gavish, J. Jones, Z. Xu, A. Christlieb, and K. Promislow, *Variational models of network formation and ion transport: applications to perfluorosulfonate ionomer membranes*, *Polymers*, 4:630–655, 2012.
- [13] H. Gomez and T.J.R. Hughes, *Provably unconditionally stable, second-order time-accurate, mixed variational methods for phase-field models*, *J. Comput. Phys.*, 230:5310–5327, 2011.
- [14] J. Guo, C. Wang, S. Wise, and X. Yue, *An  $H^2$  convergence of a second-order convex-splitting, finite difference scheme for the three-dimensional Cahn–Hilliard equation*, *Commun. Math. Sci.*, 14(2):489–515, 2016.
- [15] Y. He, Y. Liu, and T. Tang, *On large time-stepping methods for the Cahn–Hilliard equation*, *Appl. Numer. Math.*, 57:616–628, 2007.
- [16] B. Li and J.G. Liu, *Thin film epitaxy with or without slope selection*, *Euro. J. Appl. Math.*, 14:713–743, 2003.
- [17] D. Li, *On a frequency localized Bernstein inequality and some generalized Poincaré-type inequalities*, *Math. Res. Lett.*, 20(5):933–945, 2013.
- [18] D. Li, Z. Qiao, and T. Tang, *Characterizing the stabilization size for semi-implicit Fourier-spectral method to phase field equations*, *SIAM J. Numer. Anal.*, 54:1653–1681, 2016.
- [19] D. Li, Z. Qiao, and T. Tang, *Gradient bounds for a thin film epitaxy equation*, *J. Diff. Eqns.*, 262:1720–1746, 2017.
- [20] D. Li and Z. Qiao, *On Second Order Semi-implicit Fourier Spectral Methods for 2D Cahn–Hilliard Equations*, *J. Sci. Comput.*, 70: 301–341, 2017.
- [21] F. Liu and J. Shen, *Stabilized semi-implicit spectral deferred correction methods for Allen–Cahn and Cahn–Hilliard equations*, *Math. Methods Appl. Sci.*, 38(18):4564–4575, 2015.
- [22] Z. Qiao, Z. Zhang, and T. Tang, *An adaptive time-stepping strategy for the molecular beam epitaxy models*, *SIAM J. Sci. Comput.*, 33(3):1395–1414, 2011.
- [23] C.B. Schönlieb and A. Bertozzi, *Unconditionally stable schemes for higher order inpainting*, *Commun. Math. Sci.*, 9(2):413–457, 2011.

- [24] J. Shen and X. Yang, *Numerical approximations of Allen–Cahn and Cahn–Hilliard equations*, *Discrete Contin. Dyn. Syst. A*, 28:1669–1691, 2010.
- [25] J. Shen, C. Wang, X. Wang, and S.M. Wise, *Second-order convex splitting schemes for gradient flows with Ehrlich–Schwoebel type energy: application to thin film epitaxy*, *SIAM J. Numer. Anal.*, 50(1):105–125, 2012.
- [26] J. Shen and X. Yang, *Decoupled energy stable schemes for phase-field models of two-phase complex fluids*, *SIAM J. Sci. Comput.*, 36(1):B122–B145, 2014.
- [27] J. Shen and X. Yang, *Decoupled, energy stable schemes for phase-field models of two-phase incompressible flows*, *SIAM J. Numer. Anal.*, 53(1):279–296, 2015.
- [28] Z.Z. Sun, *A second-order accurate linearized difference scheme for the two-dimensional Cahn–Hilliard equation*, *Math. Comput.*, 64(212):1463–1471, 1995.
- [29] C. Wang, S. Wang, and S.M. Wise, *Unconditionally stable schemes for equations of thin film epitaxy*, *Disc. Contin. Dyn. Sys. Ser. A*, 28:405–423, 2010.
- [30] C. Xu and T. Tang, *Stability analysis of large time-stepping methods for epitaxial growth models*, *SIAM J. Numer. Anal.*, 44(4):1759–1779, 2006.
- [31] Z. Zhang and Z. Qiao, *An adaptive time-stepping strategy for the Cahn–Hilliard equation*, *Commun. Comput. Phys.*, 11:1261–1278, 2012.
- [32] J. Zhu, L.-Q. Chen, J. Shen, and V. Tikare, *Coarsening kinetics from a variable-mobility Cahn–Hilliard equation: Application of a semi-implicit Fourier spectral method*, *Phys. Rev. E*, 60(3):3564–3572, 1999.